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Electronic transport features of MoTe₂ caused by quenching

V V Marchenkov^{1,2}, A N Domozhrova¹, S V Naumov¹, S M Podgornykh¹,
V V Chistyakov¹, P S Korenistov¹ and J C A Huang³

¹M.N. Mikheev Institute of Metal Physics, UB RAS, 620108 Ekaterinburg, Russia

²Ural Federal University, 620002 Ekaterinburg, Russia

³National Cheng Kung University, 70101 Tainan, Taiwan

Abstract. The electro- and magnetoresistivity of MoTe₂ single crystals before and after quenching were measured at temperatures from 1.8 to 300 K and in magnetic fields of up to 9 T. It was demonstrated that quenching can lead to strong changes in values of the electro- and magnetoresistivity studied as well as in their temperature and field dependences. The peculiarities of these electronic transport characteristics changes were studied in detail.

1. Introduction

Transition metal dichalcogenides (TMDs) are currently believed to be very promising materials for optoelectronics, nanoelectronics and spintronics [1]. TMDs are a large group of compounds with the chemical formula MX_2 , where M is a transition metal and X is a chalcogen. These materials have very diverse properties within the TMD-group, in particular, WTe₂ and MoTe₂ in Td -phase (or γ -phase) are known to exhibit the properties of II-type topological Weyl semimetals (TWSs). TWSs are characterized by the presence of massless Weyl fermions in their bulk and Fermi arcs on the surface. Such massless quasiparticles can be controlled faster than the conventional carriers, which is promising for creating ultrafast electronic devices. At the same time, the crystal structure of MoTe₂ and its electronic characteristics, in particular, the electrical resistivity, are known to strongly depend on the heat treatment [2, 3]. Thus, in the “commonly” synthesized MoTe₂ compound, it exhibits the semiconductor characteristics: high values of the electrical resistivity and a “semiconductor” type of its temperature dependence $\rho(T)$, i.e. ρ decreases with T . Quenching leads to the fact that the value of the electrical resistivity decreases significantly, and $\rho(T)$ becomes the “metallic” one, increasing with temperature [2-4]. In addition, investigating the effect of a magnetic field on the electronic properties of these materials is of interest since a number of such papers is scarce. Therefore, the aim of this work is to study in detail the features of the electro- and magnetoresistivity of MoTe₂ before and after quenching.

2. Materials and Methods

MoTe₂ single crystals were grown by the chemical vapour transport method using Br₂ as a transport agent [3, 5, 6]. MoTe₂ is known to undergo a transition from the diamagnetic semiconductor phase to the paramagnetic metal one under certain conditions. The transition temperatures are 820°C and 880°C for tellurium-rich and molybdenum-rich samples, respectively [3]. Therefore, in order to change the type of conductivity, some single crystals were quenched from temperature above 880°C. For this purpose, some single crystals were placed into a quartz ampoule, which was evacuated to 10⁻⁴ atm. and sealed, then heated to 910°C, held at this temperature for 3 hours, and quenched in water. Figure 1 shows X-ray diffraction patterns of MoTe₂ single crystals taken from the surface ((00 \bar{l}) plane) before



and after quenching. The parameter c is seen to noticeably change after quenching from ~ 13.93 Å for the as-grown single crystal to ~ 13.81 Å for the quenched one. Note that the values of parameter c before and after quenching are close to the values of parameter c for α -MoTe₂ (hexagonal modification) and β -MoTe₂ (monoclinic modification), respectively [7-9]. The change in the parameter c , as well as the change in the ratio of the line intensities from the (00 l) planes, may indicate the structural transition that occurred during quenching.

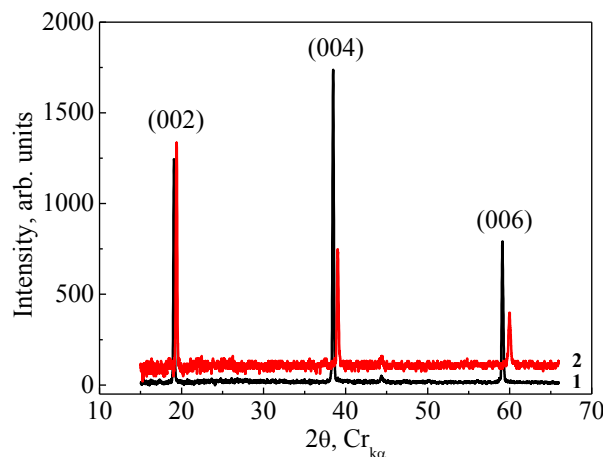


Figure 1. Fragments of X-ray diffraction patterns taken from the surface of as-grown (1) and quenched (2) MoTe₂ single crystals.

The chemical composition of the samples was confirmed by X-ray microanalysis using a FEI Inspect F scanning electron microscope equipped with an EDAX attachment. The temperature and field dependences of the resistivity $\rho(T)$ were measured by the standard four-contact method (see, e.g., Refs [10, 11]) in the temperature range from 1.8 to 300 K in magnetic fields of up to 9 T. The current and potential leads were spot welded and / or glued with silver conductive paste to the samples [12, 13]. The measurements were carried out using the PPMS-9 system (Quantum Design) in Collaborative Access Center "Testing Center of Nanotechnology and Advanced Materials" of IMP, UB of RAS.

3. Results and Discussions

Figure 2 shows the temperature dependences of the electroresistivity $\rho(T)$ of MoTe₂ before (a) and after (b) quenching in the temperature range from 1.8 to 300 K. The dependence $\rho(T)$ before quenching (figure 2a) demonstrates a "semiconductor" behaviour with a very large resistivity value of more than 10^5 Ohm·cm at low temperatures, while the resistivity is less than 1 Ohm·cm in the temperature range 50–300 K. As can be seen from figure 2b, quenching leads to a drastic change in the behaviour and value of the electrical resistivity. The temperature dependence $\rho(T)$ of MoTe₂ after quenching shows a "metallic" type with a resistivity value of $\sim (1.1\text{--}6.8)$ mOhm·cm. That is, the electroresistivity values of single crystals before and after quenching differ by 8 orders of magnitude (!) at low temperatures.

The analysis of the temperature dependences of the electroresistivity shows that $\rho(T)$ decreases exponentially with increasing temperature to ~ 100 K with characteristic temperatures $T_1 \approx 99$ K and $T_2 \approx 167$ K (see inset in figure 2a). Moreover, the "activation mode" changes at $T \sim 16$ K. An electronic transition is assumed to occur at this temperature, but additional studies are required to verify it [14]. The electroresistivity of the quenched crystal increases quadratically with temperature from the lowest T to ~ 37 K, which may be associated with the electron–electron interaction, and then linearly to ~ 70 K, which can be explained by the predominance of the electron–phonon contribution (see [15] and Refs. therein), with a further tendency to saturation. The last type of the dependence was observed in Ref. [16] in intermetallic compounds with weak static disorder and a large electron–phonon coupling constant (see also [17] and Refs. therein). However, the scattering mechanisms leading to the observed dependences $\rho(T)$ of MoTe₂ after quenching also requires a more detailed study.

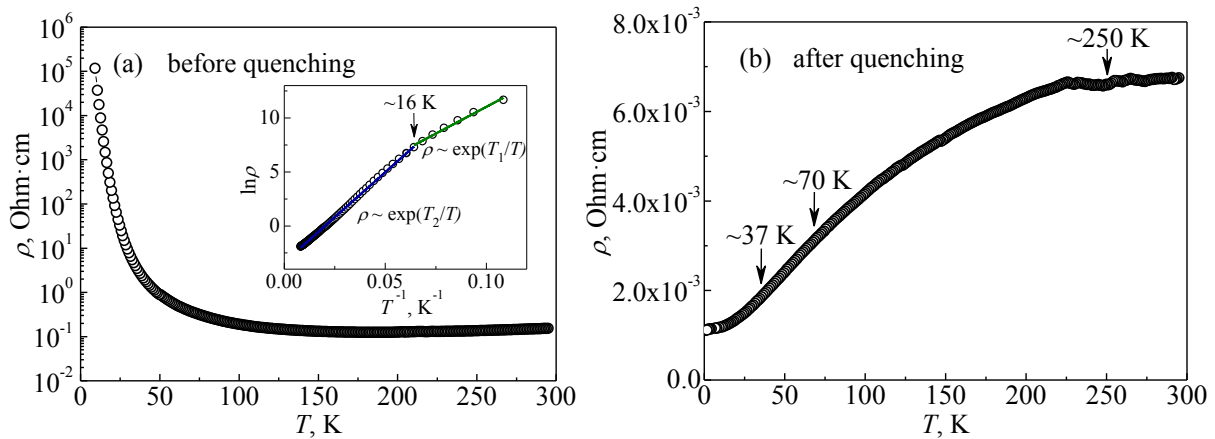


Figure 2. The temperature dependences of the electroresistivity of MoTe₂ before quenching in semilogarithmic coordinates (a) and after quenching (b). Insert in figure 2a shows the dependence $\ln \rho = f(1/T)$ of the non-quenched sample, where the arrow at ~ 16 K indicates a transition from the “low-temperature” to “high-temperature” activation mode. The vertical arrow at ~ 250 K in figure 2b indicates a structural phase transition from monoclinic modification to orthorhombic one.

The type of field dependences of magnetoresistivity (MR) is known [18] to be largely determined by the Fermi surface (FS) topology of a crystal and the state of its compensation, i.e. a ratio between the volumes of electron and hole sheets of FS. That is, crystals with the same topology of FS and state of compensation should have a similar type of field dependences of MR. Therefore, the field dependences of the MR were measured. Figure 3 shows the field dependences of the MR of MoTe₂ before (a) and after (b) quenching in magnetic fields of up to 9 T at temperatures of 12 K and 150 K. The MR was calculated by the formula

$$\Delta \rho_{xx} / \rho_0 = (\rho_{xx} - \rho_0) / \rho_0 \times 100\%, \quad (1)$$

where ρ_0 is the electrical resistivity without a magnetic field, and ρ_{xx} is the resistivity in a magnetic field.

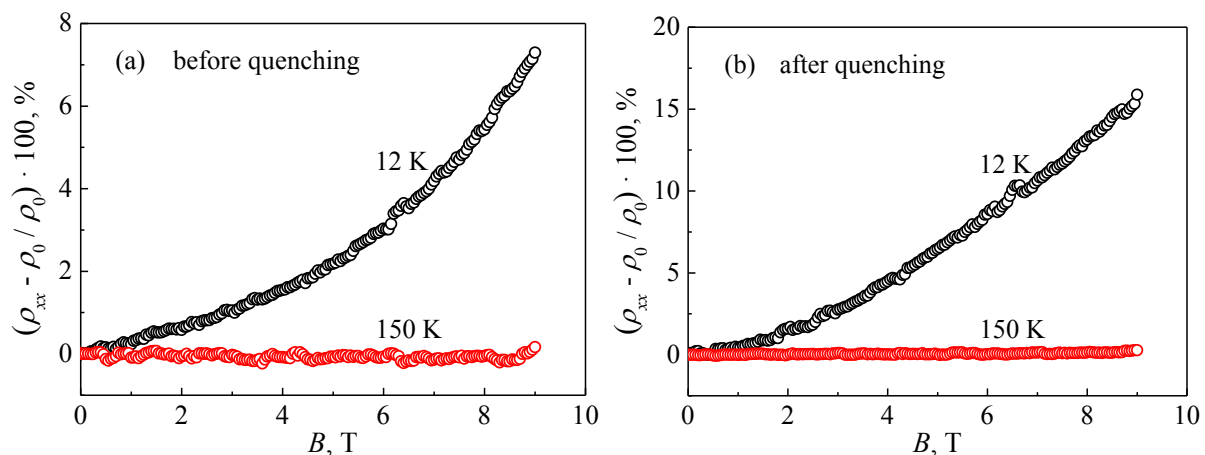


Figure 3. The field dependences of the magnetoresistivity of MoTe₂ before (a) and after (b) quenching at temperatures of 12 K (black circles) and 150 K (red circles).

Analyzing the field dependences of the MR at low temperatures, the dependence of non-quenched MoTe₂ is shown to be close to quadratic one and about 7% at $T = 12$ K in a field of $B = 9$ T. This type of $\rho(B)$ is characteristic of compensated conductors with a closed FS [18]. Quenching leads to an increase in the MR up to 15% ($T = 12$ K, $B = 9$ T), and along with the quadratic field contribution, the linear term also appears. The linear on a magnetic field contribution to the magnetoresistivity can be due to the appearance of open electron orbits perpendicular to the direction of the electric current in k -space [18]. With increasing temperature, the MR decreases and becomes less than 1% at $T = 150$ K, and its field dependence becomes close to a linear behavior for both samples. It is apparently caused by a transition to the region of effective weak magnetic fields [18], when $\omega_c \tau \ll 1$, where ω_c is the Larmor precession frequency, and τ is the relaxation time of conduction electrons.

4. Conclusions

Quenching MoTe₂ single crystals was shown to lead to the dramatic changes in the electro- and magnetoresistivity. It was observed that the resistivity value decreases up to 8 orders of magnitude (!) at low temperatures and the type of its temperature dependence changes from “semiconductor” to “metallic” one. At low temperatures, $\rho(T)$ of the non-quenched crystal was shown to change exponentially with characteristic temperatures $T_1 \approx 99$ K and $T_2 \approx 167$ K in the temperature ranges 9-16 K and 16-110 K, respectively. The electroresistivity of the quenched crystal is determined by the contributions from the scattering mechanisms of charge carriers predominating in a particular temperature range. The magnetoresistivity, which is positive for both samples, is also modified, although these changes are not so huge as in the case of the electroresistivity. At low temperatures, the magnetoresistivity of the non-quenched crystal increases quadratically with increasing magnetic field. Quenching leads to the additional linear on a magnetic field contribution to the magnetoresistivity, which can be caused by the appearance of open electron orbits. The magnetoresistivity decreases with increasing temperature, reaching $\sim 1\%$ in a field of 9 T, and has the weak linear dependence on a magnetic field.

Acknowledgments

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